LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

UCRL-PROC-213541

Missing and Spurious Level Corrections for Nuclear Resonances

G. E. Mitchell, U. Agvaanluvsan, M. P. Pato, J. F. Shriner, Jr.

July 13, 2005

International Conference in Contemporary Physics
Ulaanbaatar, Mongolia
August 8, 2005 through August 15, 2005

Missing and Spurious Level Corrections for Nuclear Resonances

G. E. Mitchell*
Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-8202
Triangle Universities Nuclear Laboratory, Durham, North Carolina 27708-0308

U. Agvaanluvsan†
L-414, Lawrence Livermore National Laboratory,
7000 East Ave., Livermore, California 94551

M. P. Pato‡
Insituto de Física, Universidade São Paulo, C.P. 66318, 05315-970 São Paulo, Brazil

J. F. Shriner, Jr.§
Department of Physics, Tennessee Technological University, Cookeville, Tennessee 38505

Neutron and proton resonances provide detailed level density information. However, due to experimental limitations, some levels are missed and some are assigned incorrect quantum numbers. The standard method to correct for missing levels uses the experimental widths and the Porter-Thomas distribution. Analysis of the spacing distribution provides an independent determination of the fraction of missing levels. We have derived a general expression for such an imperfect spacing distribution using the maximum entropy principle and applied it to a variety of nuclear resonance data. The problem of spurious levels has not been extensively addressed.

PACS numbers: 21.10.Ma,24.60.Ky,24.60.Dr,25.40.Ny

I. INTRODUCTION

Nuclear level densities are extremely important for a wide variety of phenomena, ranging from nuclear astrophysics to radiochemical applications for stewardship science. The classic method to determine level densities is by direct counting of compound nuclear states. A key difficulty is that the experiments are never perfect – some levels are not observed, and the quantum numbers of some levels are misassigned. These are usually called the missing level and spurious level problems. The solutions – that is, the attempts to complete and/or to purify the data sets – all assume that the underlying distributions obey the Gaussian Orthogonal Ensemble (GOE) version of Random Matrix Theory (RMT).

For the missing level problem, the standard approach assumes (1) that the underlying strength distribution is a Porter-Thomas (PT) distribution [1] and (2) that all of the levels with strengths below some threshold value are missed and that all of the levels with strengths above the cutoff value are observed. From the observed (incomplete) PT distribution, the fraction of missing levels is determined. This method works well as long as the behavior is purely statistical. Non-statistical phenomena (e.g., doorway states) can have a major impact on the observed distribution and lead to an incorrect missing level correction. We have developed a method that uses the measured spacing distributions (for which the effects of non-statistical phenomena are minimal) to determine the missing level correction [2, 3]. In RMT the spacings are independent of the widths and thus can provide independent tests for missing and spurious levels. Using the principle of maximum entropy, we have obtained the probability distribution for imperfect eigenvalue sequences. The derivation of this distribution is summarized in Section II. Recently Bohigas and Pato [4] have generalized our results.

The spurious level problem has generally been treated very differently than the missing level problem: the focus for spurious levels has been on whether or not an *individual* level belongs to the primary data set under consideration, rather than the *overall* characterization of the data set. For instance, in the standard neutron total cross section measurements, there is no clear signature that indicates the resonance ℓ or J value. To determine the ℓ value a Bayesian probabilistic approach is used [5]. This method is based on the fact that (for low energy neutron resonances) the difference in penetrabilities for s- and p-wave resonances is large, and thus the means of the PT distributions for the two types of resonances are very different. This method works well in general, but is not reliable near the *a priori* probability value that divides the s- and p-wave resonances: strong p-wave resonances and weak s-wave resonances are often misidentified and are therefore likely to result

*Electronic address: mitchell@tunl.duke.edu
†Electronic address: agvaanluvsan1@llnl.gov
‡Electronic address: mpato@uspif1.if.usp.br
§Electronic address: jshriner@tntech.edu

in spurious levels. Non-statistical effects may also distort the analysis.

We adopted a simple test that returns the focus to individual levels. The most striking characteristic of the nearest-neighbor spacing distribution is level repulsion. Since states of the same symmetry only rarely occur very close together, one can use small experimental spacings as a signature of spurious levels. One of the two levels used to determine the anomalous spacing is likely to be spurious. We have quantified this simple approach and applied it to resonance data. [6]

II. STANDARD WIDTH CORRECTION METHOD

The Gaussian assumption for the distribution of reduced width amplitudes leads to the Porter-Thomas distribution for the dimensionless strength parameter y:

$$P(y) = \frac{1}{\sqrt{2\pi y}} e^{-\frac{y}{2}}, \tag{1}$$

where $y \equiv \gamma^2/\langle\gamma^2\rangle$, γ^2 is the reduced width, and $\langle\gamma^2\rangle$ is the average reduced width. One assumes that all levels weaker than the weakest observed level are missed and that all levels with larger widths are observed. A modified PT distribution was introduced by Fröhner [7]:

$$P_F(y) = \begin{cases} 0 & : \ y < y_0 \\ \dfrac{1}{\mathrm{erfc}\left(\sqrt{y_0/2}\right)} \dfrac{\mathrm{e}^{-y/2}}{\sqrt{2\pi y}} & : \ y \geq y_0 \end{cases} \tag{2}$$

The term involving the complementary error function ensures that the distribution is normalized to a total probability of one. Maximizing the likelihood function constructed from the modified PT distribution yields the equation

$$\langle\gamma^2\rangle = \langle\gamma^2\rangle_{obs}\Big(1 + \sqrt{\frac{2y_0}{\pi}} \frac{e^{-y_0/2}}{\mathrm{erfc}\sqrt{y_0/2}}\Big)^{-1}. \tag{3}$$

The solution to this equation can be obtained iteratively as described in Ref. [3] and yields the most likely value for the average reduced width $\langle\gamma^2\rangle$; that in turn can be used to determine the observed fraction of levels f.

This method works fairly well in the absence of non-statistical effects. However, if non-statistical effects such as doorway states are present, the result is that the average value of the reduced widths is overestimated and the cutoff parameter y_0 is therefore too small. If the non-statistical effect is well understood, then it can be quantified and removed from the data set before analysis. However, even in favorable cases this is often difficult to achieve, and in many cases the origin of the anomaly is not understood. In order to improve the reliability of the analysis and to provide an independent test, we developed a method based on the spacing distribution.

III. NEW SPACING CORRECTION METHOD

The energies of nuclear resonances with the same quantum numbers form a GOE eigenvalue sequence. The nearest-neighbor spacings of perfect GOE sequences are to a good approximation described by the Wigner distribution [8]

$$P_{GOE}(x) = \frac{\pi x}{2} \mathrm{e}^{-\pi x^2/4}, \tag{4}$$

where $x \equiv S/D$, S is a spacing between adjacent levels and D is the average spacing. We need the spacing distribution of an incomplete (imperfect) sequence. Because the positions of missing levels are random, the spacing distribution is affected by missing levels in a more complicated way than is the width distribution.

Some of the nearest-neighbor levels in the imperfect sequence are not actual nearest neighbors, due to missing levels between the observed levels. Thus the nearest-neighbor spacing distribution for the imperfect sequence reflects the presence of higher order spacing distributions. The observed nearest-neighbor spacing distribution (NNSD) for an imperfect sequence can be written as

$$P(z) = \sum_{k=0}^{\infty} a_k \lambda P(k; \lambda z). \tag{5}$$

The parameter z is defined as $z \equiv fx$, where f is the observed fraction of levels ($f = N_{observed}/N_{true}$). The parameters a_k give the relative contributions of the k-th nearest-neighbor spacing distributions $P(k; \lambda z)$. λ is a parameter that characterizes the incompleteness of the sequence.

The detailed derivation of the NNSD for imperfect sequences is given in [3]. Here we present only a brief outline of the derivation. We require that the distribution $P(z)$ has total probability 1 and that the average value of z is 1. The functions $P(k; \lambda z)$ also must be normalized to 1 and must have an average value $k + 1$ when expressed in terms of the variable x. Combining these relations yields two constraints:

$$\begin{aligned} \sum_{k=0}^{\infty} a_k &= 1, \\ \sum_{k=0}^{\infty} a_k (k+1) &= \lambda. \end{aligned} \tag{6}$$

To determine the coefficients a_k we define an entropy

$$S\{a_k\} = -\sum_{k=0}^{\infty} a_k \ln a_k. \quad (7)$$

We wish to find the values $\{a_k\}$ that maximize S subject to the constraints in Eqs. (6). We utilize two Lagrange multipliers α and β to account for the two constraints. Maximizing the entropy requires that

$$\delta\{-\sum_{k=0}^{\infty} a_k \ln a_k - \alpha \sum_{k=0}^{\infty} a_k - \beta \sum_{k=0}^{\infty} (k+1) a_k\} = 0. \quad (8)$$

The values that maximize the entropy are $a_k = f(1-f)^k$ and $\lambda = 1/f$.

Combining these results yields the final expression

$$P(x) = \sum_{k=0}^{\infty} f(1-f)^k P(k;x). \quad (9)$$

This result is general and therefore applies to any of the ensembles of RMT. To choose a particular ensemble requires specifying the appropriate $P(k;x)$ for that ensemble. P(0;x) is the Wigner distribution, P(1;x) and P(2;x) are determined by interpolations of numerical data and $P(k;x)$ for $k \geq 3$ are approximated by Gaussians centered at $k+1$ with the appropriate variances. Although we have worked out the details for all three of the standard Gaussian ensembles (Orthogonal, Unitary, and Symplectic), with one exception our applications have all been to nuclear resonances and the GOE version of RMT.

Since the spacing analysis was new and thus unproven, we tested the analysis method on numerically generated data with very good statistics. To test the spacing distribution function we generated GOE sequences and then randomly removed a fraction 1 - f of the levels. We used the maximum likelihood method – the likelihood function is $L = \Pi_i P(x_i)$, where the product is over all spacings in the sequence. The most probable value of f is the one that maximizes the likelihood function, and the uncertainty in f is the deviation from the most likely value of f when ln L has decreased by 0.5 from its maximum value. These tests led to excellent agreement with the known values of missing levels.

IV. COMPARISON WITH DATA

We first considered data that our group had previously measured; we examined a sequence of proton resonances in ^{48}Ti(p,p) with spin and parity $1/2^+$. These data were considered to be of high quality and displayed no anomalous effects. We analyzed these data with both the standard width correction method and the new spacing correction method. The results were $f_{width} = 0.87^{+0.13}_{-0.11}$ and $f_{spacing} = 0.88 \pm 0.07$. The results were in excellent agreement with each other and led to a weighted average value of $f = 0.88 \pm 0.06$. Even in this case where the two methods agreed very well with each other, the result is a value in which there is greater confidence and has a smaller uncertainty.

The presence of non-statistical effects has a severe impact. The additional strength added to the (true) background strength by a doorway state may significantly increase the average reduced width $\langle\gamma^2\rangle$, and thus incorrectly decrease the cutoff value y_0. The net result is that the number of missing levels in underestimated. Of course if one knows the nature of the non-statistical effect, then this contribution can be evaluated and subtracted before performing the missing level analysis.

In practice this works reasonably well for proton resonances where the non-statistical effects are isobaric analog states.[6] However, a major problem arises for neutron resonances. There are many non-statistical effects observed in neutron resonances, but there is no formal prescription that enables one to extract a reliable value for the strength of the non-statistical effect. Even its existence may be in question. Due to the nature of the Porter-Thomas width distribution, it is sometimes difficult to distinguish between an unusually large width and a true non-statistical effect. The precise amount of strength to assign to the non-statistical anomaly is even more difficult to determine. Thus the main advantage of the spacing analysis is for neutron resonances with possible doorways.

We illustrate this with data from the n + ^{238}U reaction. We consider 237 s-wave resonances identified by Olsen *et al.* [9, 10]. The reduced width distribution is shown in Fig 1. Analysis using the width correction method for the missing levels yields $f = 0.97^{+0.03}_{-0.08}$. The data are considered to be essentially perfect, although the bulge in the integral plot is somewhat suspicious.

We then analyzed these same ^{238}U resonances with the spacing correction method. The spacing distribution and its integral are shown in Fig. 2. The spacing analysis method yields a value of $f = 0.89 \pm 0.06$.

The question is which of these two methods to believe – are the data essentially perfect (as implied by the width correction method) or are there approximately 10% missing levels? A very strong indication of which to choose is provided by inspection of the spacing distribution in Fig. 2. There are a number of observed spacings greater than $x = 3$ and some even greater than $x = 4$. However, for the Wigner distribution, the probability of $x \geq 3$ is 0.001 and the probability of $x \geq 4$ is much much lower! By inspection there must be a number of missing levels. Comparison with numerical simulations for various values of f suggest that an f value of about 0.9 is quite rea-

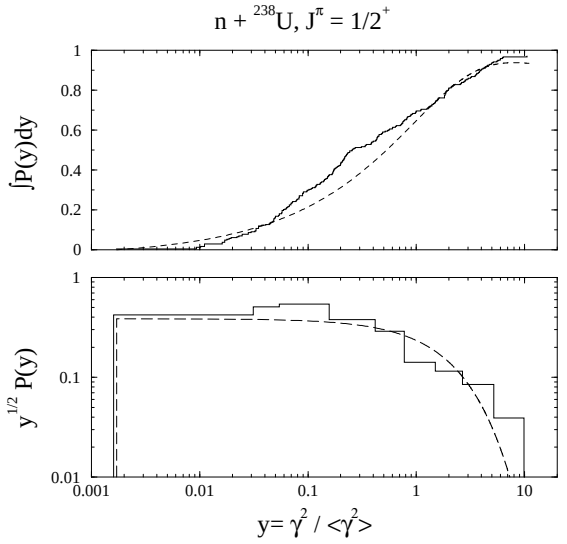

FIG. 1: Reduced width distribution for $1/2^+$ resonances in the n + ^{238}U reaction. The dashed lines show the truncated PT distribution for $f = 0.97$.

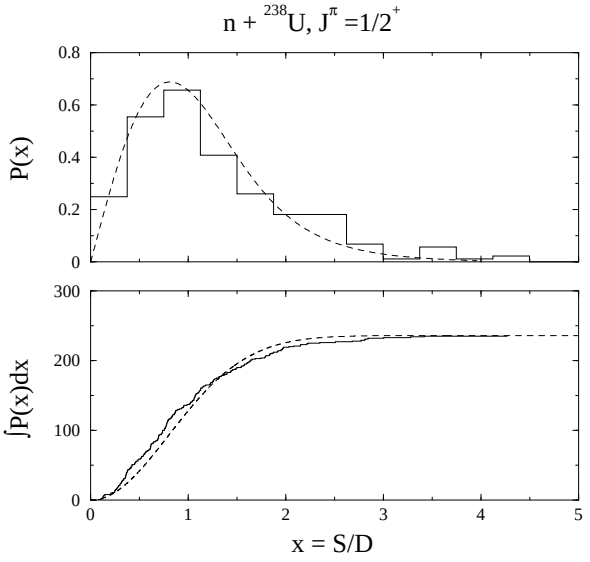

FIG. 2: Nearest-neighbor spacing distribution for $1/2^+$ resonances in the n + ^{238}U reaction. The dashed lines show the expected behavior for $f = 0.89$

sonable. Performing the missing level correction with both methods should significantly reduce errors that result from non-statistical effects.

V. SUMMARY AND CONCLUSIONS

Assuming that the nuclear resonances behave statistically and that Random Matrix Theory describes their behavior, then one can analyze either the width or the spacing distribution in order to determine the missing fraction of levels. Since the weakest levels are missed systematically, the width correction method is simple and transparent. The observed spacing distribution is a weighted sum of the probability distributions for two levels that have no levels between them – $P(0;x)$, one level between them – $P(1;x)$, etc. With the maximum entropy principle a general expression for the imperfect eigenvalue distribution was obtained. Practical approximations for the $P(k;x)$ were obtained. In practice the spacing correction method works very well. The advantage of this method is striking when non-statistical effects are present, since the spacing distribution is not affected by the presence of doorway states. Thus the new correction method provides at a minimum an additional method that helps to confirm the reliability of the data and to reduce the uncertainty in the value of the missing level correction. In extreme cases this new method prevents serious errors in estimating the fraction of missing levels.

These efforts were directed at determining the fraction of missing levels in the experimental spacing distribution. An equally interesting and even more challenging problem is that of determining whether a given state belongs in the sequence or whether there is a specific level missing between two given levels. That is, what is the information content of a state in a correlated sequence? Consider two extremes: for a picket fence distribution one can tell with 100% certainty that a state is missing. On the other hand for a Poisson distribution, if a state is missing, then the observer has no information. Any correlated sequence such as the RMT ensembles are somewhere in between these two extremes.

Dyson and Mehta [11, 12] developed a statistical mechanics of correlated spectra and obtained specific values for many thermodynamic variables (internal energy, specific heat, entropy, ...) for the three basic RMT ensembles. This topic has not been considered either theoretically or experimentally. As a outgrowth of our present efforts, we initiated efforts to examine what can be called RMT thermodynamics. The initial results are presented in the next paper [13].

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Department of Energy under grants Nos. DE-FG02-97-ER41042, DE-FG02-96-ER40990, and DE-FG03-03NA00076, by the U.S. National Science Foundation under grant No. INT-0112421, and by the Fundação de Amparo a Pesquisa do Estado de São Paulo (FAPESP). Part of this work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory, under contract No.

W-7405-Eng-48.

[1] C. E. Porter and R. G. Thomas, Phys. Rev. **104**, 483 (1956).
[2] U. Agvaanluvsan, Ph.D. thesis, North Carolina State University (2002).
[3] U. Agvaanluvsan, G. E. Mitchell, J. F. Shriner, Jr., and M. Pato, Nucl. Instrum. Methods **A498**, 459 (2003).
[4] O. Bohigas and M. P. Pato, Phys. Lett. B **595**, 171 (2004).
[5] L. M. Bollinger and G. E. Thomas, Phys Rev **171**, 1293 (1968).
[6] S. J. Lokitz, G. E. Mitchell, and J. F. Shriner Jr., Phys. Rev. C **(to be published)**, (2005).
[7] F. Fröhner, in *Nuclear Theory for Applications* (IAEA, Vienna, 1980), vol. IAEA-SMR-43, p. 59.
[8] E. P. Wigner, in *Statistical Theories of Spectra: Fluctuations*, edited by C. E. Porter (Academic Press, New York, 1965), p. 199.
[9] D. K. Olsen, G. de Saussure, R. B. Perez, F. C. Difilippo, R. W. Ingle, and H. Weaver, Nucl. Sci. Eng. **69**, 202 (1979).
[10] D. K. Olsen, Nucl. Sci. Eng. **94**, 102 (1986).
[11] F. J. Dyson and M. L. Mehta, J. Math. Phys. **4**, 701 (1963).
[12] M. L. Mehta, *Random Matrices* (Academic, New York, 1991), 2nd ed.
[13] M. P. Pato et al., This conference.